

# Mechanics of solid materials

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# 1

## ELEMENTS OF THE PHYSICAL MECHANISMS OF DEFORMATION AND FRACTURE

*Lorsqu'un théoricien trouve un résultat nouveau personne n'y croit,  
sauf lui! lorsqu'un expérimentateur trouve un résultat nouveau tout  
le monde y croit, sauf lui!*

The aim of this first chapter is to give nonspecialists in physics and metallurgy a general idea of the structure and mechanisms of deformations and fracture of the principal materials used in ordinary structures. Therefore, it consists of a brief summary of the classical knowledge as found in specialized works. The main references among these are given in the bibliography. Knowledge of these basic physical mechanisms is necessary for the formulation of hypotheses upon which the macroscopic phenomenological theories of deformation and fracture can be based. These theories, presented in Chapters 4–8, must indeed integrate the phenomena associated with discrete entities such as atoms, crystals, molecules, cells, etc., to the level of homogeneous continuum models. In metals, the introduction of the concept of dislocations by Taylor and several others in 1934 marked the first decisive step in explaining the phenomenon of plastic deformation. In a more general way, the invention of transmission and scanning electron microscopes has permitted, during the 1960s, an understanding of the main mechanisms of deformation and fracture.

It must, however, be remembered that in the field of fracture where these phenomena occur at the much larger scale of crystal or molecular arrangements, there are several unresolved questions, and for this reason the schematic treatment given in this chapter remains very rudimentary.

Paradoxically, despite the large differences in the nature and structure of materials such as metals and alloys, polymers and composites, concrete, wood, there is a great unity displayed in their macroscopic behaviour. With different orders of magnitude, terms like elasticity, viscosity, plastic or permanent deformation, consolidation or hardening, brittle fracture and ductile fracture can be applied to all these materials. This is what justifies ‘*a priori*’ the global approach to the mechanics of materials which, with the aid

of concepts from continuum mechanics and thermodynamics in Chapter 2, and from rheology in Chapter 3, allows the construction of models independent of the nature of materials in their basic properties (but not in their analytical formulations).

## 1.1      **Metals and alloys**

### 1.1.1      *Structure*

#### *Elements of crystallography*

##### *Atoms*

Metals and alloys are made up of arrangements of atoms held together by electromagnetic forces between the electrons of neighbouring atoms. The order of magnitude of the 'radius' of an atom varies from  $10^{-7}$  to  $10^{-6}$  mm ( $1-10 \text{ \AA}$ ). Stable arrangements are determined by a minimum energy condition of the atomic packing, which is a function of thermal activation. In metals, the bonds result from a sharing of electrons in the outer shells of the atoms. Metals and alloys are normally found to consist of closely packed crystals. The amorphous state can only result from complex processes requiring extremely fast cooling.

##### *Monocrystals*

The crystalline state is characterized by the regularity of the atomic arrangement; an elementary parallelepipedic pattern or lattice repeats itself periodically in all three directions.

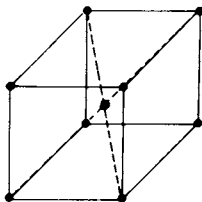
Most of the metallic lattices belong to one of the three following systems:

Cubic centred (CC) crystals (Fig. 1.1) e.g., Fe $\alpha$ , Cr, Mo

Face centred cubic (FCC) crystals (Fig. 1.2) e.g., Cu, Ag, Al, Ni

Close packed hexagonal (CPH) crystals (Fig. 1.3) e.g., Mg, Zn, Ti $\alpha$ , Co $\alpha$ .

Fig. 1.1. CC crystals.



These lattices possess axes and planes of symmetry, the latter being in general the planes in which the atoms are most densely packed and which possess a lower resistance to shear. Their conventional representation is by means of Miller indices: the plane to be characterized is identified by the coordinates of its intersection with the axes of an orthogonal reference system, with the reciprocals of these numbers reduced to the three smallest integers which have the same ratios (Fig. 1.4).

Fig. 1.2. FCC crystals.

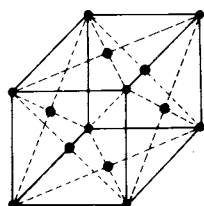


Fig. 1.3. CPH crystals.

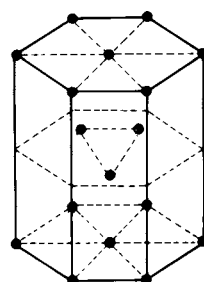
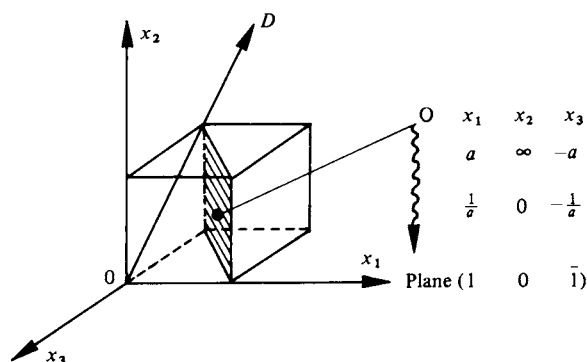


Fig. 1.4. Miller indices.



A crystallographic direction is characterized by a straight line emanating from the origin of the reference system and passing through the position of an atom. It is designated by the coordinates of that atom expressed in terms of interatomic distances. For example, the direction  $OD$  in Fig. 1.4 is expressed as  $\langle 01\bar{1} \rangle$ .

The structure of an alloy can be either that belonging to one of the constitutive elements or an entirely different crystalline structure. In solid solutions, it is possible to have the substitution of an atom from the lattice (for example aluminium in iron) or the insertion of small atoms in the network of the solvent (for example carbon in iron for austenite (Fig. 1.5)). Metals can take different forms or phases depending on the temperature. The most common phases for steels are the  $\gamma$  and  $\alpha$  phases (respectively FCC for austenite and CC for the ferrite of the carbon-iron system). It is also possible to have stable or unstable secondary phases, phases  $\beta$ ,  $\delta$ ,  $\epsilon$ ,  $\sigma$ , and in a particular phase it is possible to distinguish the cases in which the substitute atoms occur in a disordered state (for example phase  $\gamma$ ) or in an ordered state (for example phase  $\gamma'$ ).

### Polycrystals

Metals and alloys are generally produced in a liquid state, and their structure is formed as they solidify when cooled. As the temperature of the liquid decreases, the interatomic distances become smaller; the critical distance, at which bonding occurs, is reached at several, randomly distributed sites, and these constitute the first germs or nuclei of crystal growth. The lattices are formed in the same crystalline system but in random directions. Each nucleus develops into a crystal whose growth is limited by neighbouring crystals. A polycrystal is made up of several monocrystals oriented randomly. The size of such monocrystals varies from a few microns ( $10^{-3}$  mm) to a few millimetres depending on the nature of the constituent elements of the metal, as well as on the thermal and mechanical treatments to which the polycrystal has been subjected (Fig. 1.6). It is therefore

Fig. 1.5. Solid solution of substitution (S) or insertion (I).

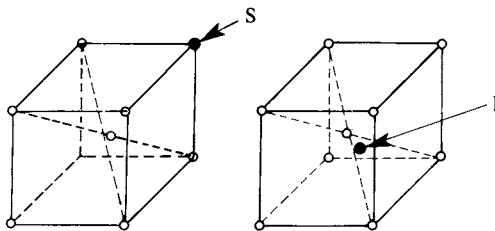
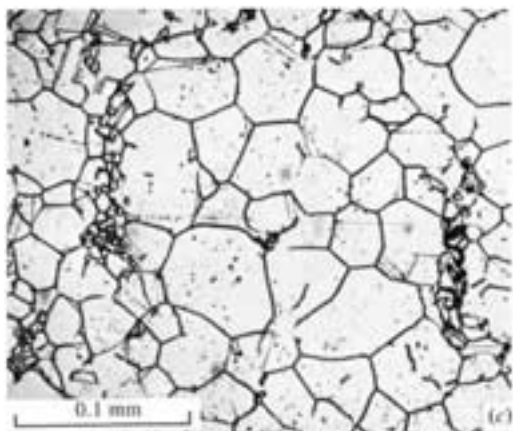
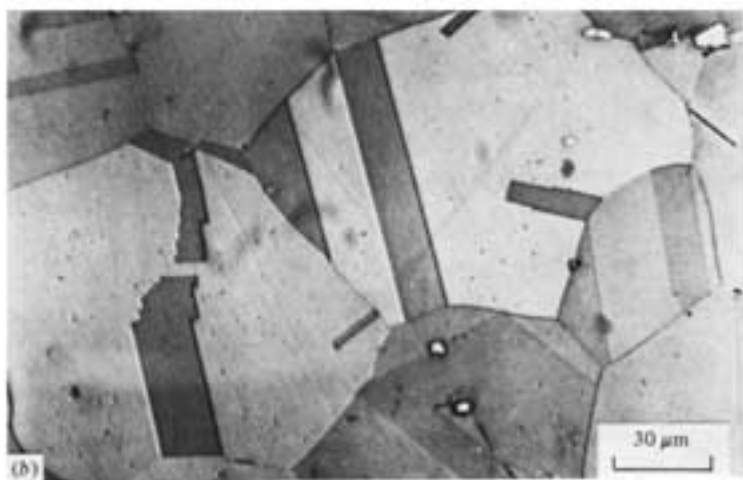
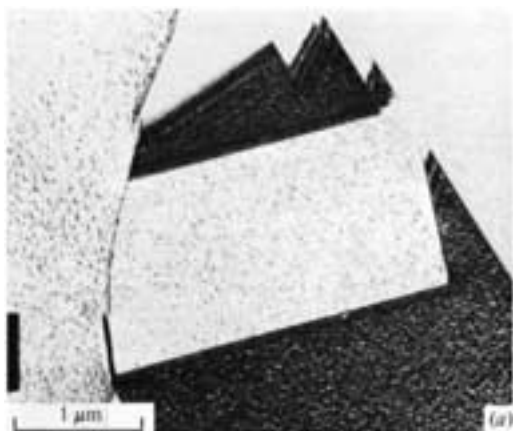


Fig. 1.6. Examples of crystals (after A. Pineau): (a) nickel based Inconel 718 alloy, transmission electron microscopy; (b) nickel Waspaloy alloy, optical microscopy; (c) nickel based Inconel 718 alloy, optical microscopy.



understandable that although a polycrystal consists of essentially anisotropic monocrystals, it can often be regarded as macroscopically isotropic, i.e., without any preferred direction for the properties under consideration.

### *Crystal defects*

The structure of the perfect crystal as described above can only account for elastic deformations and for so-called brittle fracture in which the loss of cohesion occurs without noticeable macroscopic deformation. Plastic deformations and tensile fracture can only be explained by the presence of defects that disturb the crystal lattice.

#### *Point and surface defects*

Atomic point defects consist of atoms inserted or substituted in solid solutions and of vacancies (i.e. points in the lattice where atoms are missing). They result in a local distortion of the lattice.

Surface defects are the surfaces of separation between crystals or parts of a crystal where the orientations or natures of the phases are different. Their thickness is of the order of 4–5 atomic 'diameters'. For example,

- grain boundaries (or crystal boundaries) in polycrystals,
- dislocation loops and cells,
- twin crystal boundaries,
- interfaces between two phases.

Cohesion defects, consisting of the surfaces of separation in a material which lead to fracture, are micro-cracks and cavities.

#### *Dislocations (line defects)*

These are the defects which are mainly responsible for plasticity of metals. A line of dislocation is a defect in the arrangement of atoms which is repeated periodically and which represents the equilibrium state of atoms with slightly different magnetic fields. It is possible to give a schematic representation of such defects in the case of simple cubic crystals:

- An edge dislocation or defect which would be created by the translation of the upper part of the crystal (Fig. 1.7).

- A screw dislocation or defect which would be created by a local rotation of the upper part of the crystal (Fig. 1.8).

- A dislocation loop or line which, for example, joins a pure edge dislocation to a pure screw dislocation (Fig. 1.9).

Dislocations are created during the growth of the crystals; their density, which is very high in most metals and alloys, varies from  $10^4 \text{ km cm}^{-3}$  for well-annealed crystals to  $10^7 \text{ km cm}^{-3}$  for heavily cold-worked samples. Fig. 1.10, which was obtained by scanning electron microscopy, shows a dislocation configuration. Prolonged heat treatments favour the arrangement of dislocations in the form of almost regular three-dimensional cells consisting of crystal planes and nodes, called *Frank networks*.

Fig. 1.7. Edge dislocation of line  $DC$ .

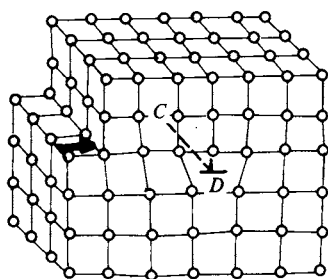


Fig. 1.8. Screw dislocation of line  $DV$ .

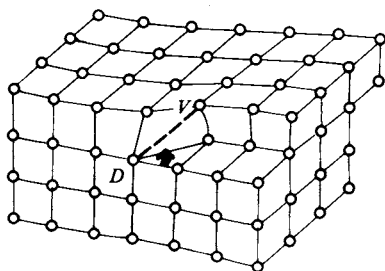
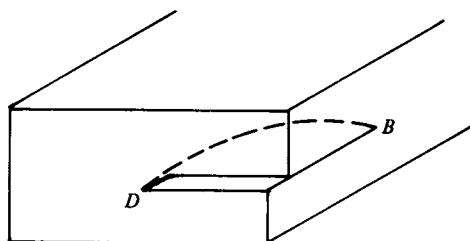


Fig. 1.9. Dislocation loop of line  $BD$ .



*Burgers vector*

A dislocation can be characterized by the 'lack of closure' vector of a contour encircling the dislocation line. Let us consider two simple cubic crystals one perfect and the other with an edge dislocation  $L$  (Fig. 1.11). In the latter, let us consider a closed loop  $ABCD$  around the point  $L$  with the sense of traverse defined with respect to an orthogonal reference system. Now let us, reproduce this contour in the perfect crystal by counting the same number of interatomic distances:  $A'B'C'D'E'$ . To close the contour, the vector  $\vec{E'A'}$  should be added. This vector by definition is the Burgers vector  $\vec{b}$ .

Burgers vectors have the following properties:

- they are independent of the contour;
- their magnitude defines the translation which would be necessary to create a dislocation;

Fig. 1.10. Dislocations in a stainless steel. Fe20 Cr–Ni–Al hardened by precipitation in the ordered phase Ni–Al (after Pineau).

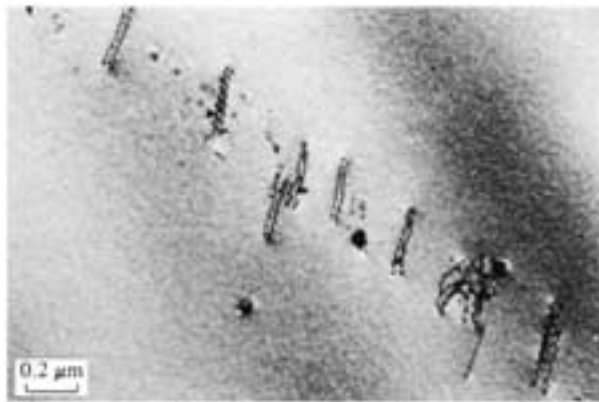
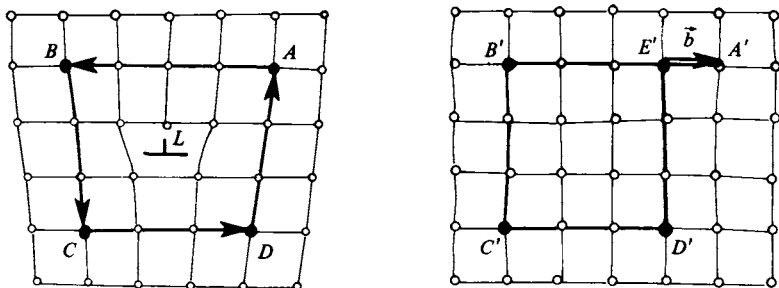


Fig. 1.11. Burgers vector.





they are constant along the whole dislocation line;

if  $\vec{\tau}$  is a unit vector on the dislocation line then:

if  $\vec{\tau}$  and  $\vec{b}$  are perpendicular to each other, the dislocation is an edge dislocation;

if  $\vec{\tau}$  and  $\vec{b}$  are parallel, the dislocation is a screw dislocation;

if  $\vec{\tau}$  and  $\vec{b}$  are at some angle to each other, the dislocation is a mixed one;

the closing vector of a contour surrounding several dislocations is the sum of the Burgers vector of these dislocations.

### *Energy associated with dislocations*

Since dislocations produce purely elastic distortions of the lattice, and since the neighbourhood of a dislocation can be considered to be a linear elastic continuum, we can calculate the elastic energy  $w_e$  stored in the material in the form of internal stresses and strains. For an edge dislocation or a screw dislocation (Fig. 1.12) of unit length and a Burgers vector of magnitude  $b$  in a medium with shear modulus  $\mu$ , we find that the stored energy is of the order of

$$w_e = \mu b^2 \text{ Jm}^{-1}.$$

In the same way, it is possible to calculate the force  $\vec{F}_D$  which would be exerted on a dislocation of unit vector  $\vec{\tau}$  and Burgers vector  $\vec{b}$  in a uniform stress field  $\sigma$ . This is the Peach-Koehler relation

$$\vec{F}_D = (\sigma \cdot \vec{b}) \wedge \vec{\tau}.$$

### 1.1.2 *Physical mechanisms of deformation*

#### *Elastic deformation*

Elastic deformations occur at the atomic level. The observed macroscopic effect is the result of the variations in the interatomic spacing necessary to balance the external loads, and also of the reversible movements of dislocations. These geometrical adjustments are essentially reversible. In a

Fig. 1.12. Energy associated with dislocations.



purely elastic deformation, the initial configuration of atoms is restored upon the removal of the load.

### *Permanent deformations*

Plastic or viscoplastic permanent deformations occur at the crystal level, and are in addition to elastic deformations; they correspond to a relative displacement of atoms which remains when the load is removed. Depending on the case, the deformations are either purely intragranular (inside the grains) or involve intergranular displacements. The ratio of joint deformation to grain deformation remains small, but it generally increases with increasing temperature and also with decreasing strain rate.

#### *Deformation by slip and twinning*

Symmetry planes of the crystal lattice, which are also the reticular planes of the most densely packed atoms, form the parallel planes with the greatest distance between them. It is therefore in these planes that slip due to shear can occur in the direction of maximum shear stress, e.g., planes (1, 1, 1) in FCC crystals; and planes (1, 1, 0) and (1, 1, 2) in the BCC crystals. They occur in the form of parallel slip bands which result in steps on the exterior surface of the samples (Fig. 1.13(a)) or in the form of twins which consist of slips symmetric with respect to a plane (Fig. 1.13(b)).

Twinning is more characteristic of deformations which occur at average or room temperature. It occurs in CC and CHP crystals in conjunction with slips, but also in FCC crystals where the energy of stacking defects is low. These defects, slips or twinings, are, in fact, heterogeneous deformations at the crystal level, but may be considered homogeneous at the macroscopic level.

#### *Deformation by dislocation movements*

The presence of dislocations considerably reduces the stability of the crystal lattice. Their mobility is the essential cause of permanent deformations, homogeneous at the macroscopic scale.

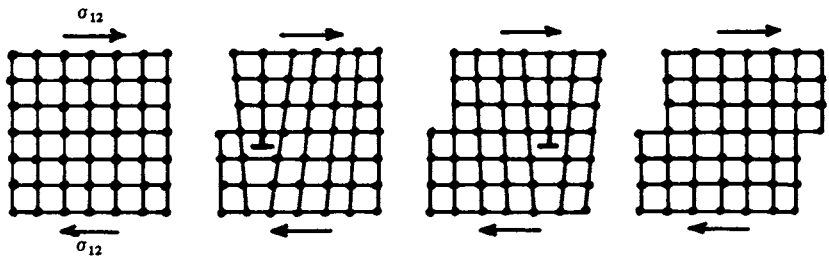
Slip displacement: when, under an external load, an edge or screw dislocation moves across a crystal, irreversible displacement occurs which is equal to the Burgers vector. Fig. 1.14 shows an edge dislocation in a cubic crystal subjected to a shear stress  $\sigma_{12}$ . The plane defined by the unit vector  $\vec{t}$  and the Burgers vector  $\vec{b}$  is called the slip plane.

This displacement mechanism requires the breaking of bonds only in the vicinity of the dislocation line, and successively from one atom to the next.

Fig. 1.13. (a) Slip bands in nickel based Waspaloy (after Pineau). (b) Twinning deformation in zinc (after Pineau).



Fig. 1.14. Slip displacement of a dislocation.



In the more complex case of a dislocation loop, the plane of the loop can digress into another plane (a perpendicular one for example) arising from its 'pure screw' point to avoid an obstacle such as an impurity; this is called a deviated slip.

**Climb displacement:** an edge dislocation can move perpendicularly to its slip plane with the transport of material. If a void is close to a dislocation line, then a distortion of the lattice resulting from the application of an external load can cause an atom of the lattice to jump by half a plane on the empty side of the crystal and result in the rearrangement of the whole row of atoms. Thus, in this mechanism, the dislocation climbs up by one interatomic space (Fig. 1.15). This displacement mechanism, linked to the diffusion of vacancies or foreign atoms, is favoured by thermal activation; it, therefore, occurs mostly at high temperatures ( $T > \frac{1}{3} T_M$ , where  $T_M$  is the melting temperature).

The rate of dislocation displacement (slip or climb) can be very low or very high depending upon the applied stress, but it cannot be higher than the speed of sound in the material under consideration.

Fig. 1.15. Climb displacement of a dislocation.

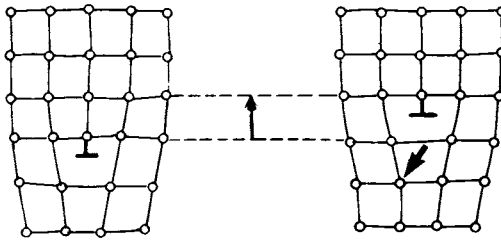
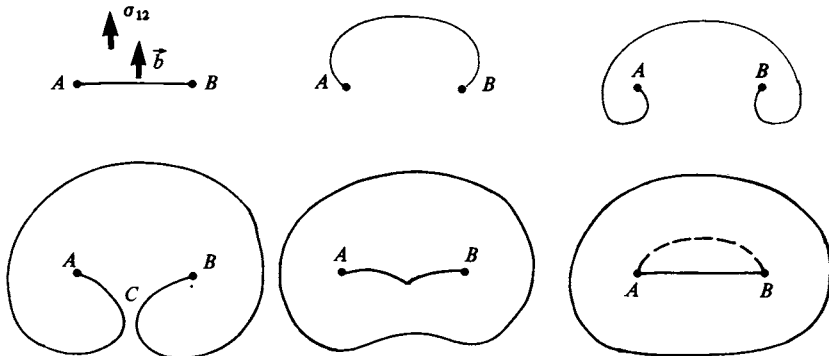


Fig. 1.16. Generation of dislocations by the Frank-Read mechanism.



*Sources of dislocations*

Dislocation movements cause permanent deformations; conversely, large plastic deformations increase the density of dislocations which, in turn, increases the number of blockings and contributes to further hardening. The most important source of dislocations is that described by the Frank–Read mechanism. Let us consider a dislocation segment anchored at  $A$  and  $B$ , the points of intersection with other dislocations or impurities (Fig. 1.16), of Burgers vector  $\vec{b}$  normal to  $AB$  and subjected to a shear stress  $\sigma_{12}$  in the same direction as  $\vec{b}$ . Under the applied stress, the dislocation is forced to move around the points  $A$  and  $B$ . When the two branches rejoin at  $C$ , they have the same Burgers vector but opposite unit vectors. They combine to create a large loop and a new segment  $AB$  which in turn generates another loop and so on...

*Elasticity limit*

It is easy to calculate the elastic limit of a perfect stack of atoms assuming that the shear stress causing one set of atoms to glide over another in a plane, is a sinusoidal function of a period equal to the interatomic distance (the Frenkel hypothesis). Assuming that in the vicinity of the equilibrium position, this shear stress is linearly related to the corresponding deformation through the shear modulus  $\mu$ , the maximum  $\tau_Y$  of this stress corresponding to the limit of reversibility of the movement is found to be

$$\tau_Y = \mu/2\pi.$$

This value is of the order of 100 times higher than the elastic limit in shear of common metals, but it is very close to the values observed for ‘whiskers’ or thin fibres which consist of perfect stacks of atoms. For example,

Theoretical elastic limit	$\left\{ \begin{array}{l} \text{pure iron} \\ \text{whiskers of iron} \end{array} \right\}$	$\tau_Y = 84700/2\pi = 13550 \text{ MPa}$
Measured elastic limit		
	$\left\{ \begin{array}{l} \text{pure iron} \\ \text{whiskers of iron} \end{array} \right\}$	$\tau_Y = 28 \text{ MPa}$ $\tau_Y = 11000 \text{ MPa}$

The elastic limit of a real single crystal is very difficult to evaluate because of the different mechanisms which can occur:

the dislocation loops generated by the Frank–Read mechanism and which emerge at the free surface of the crystal create an irreversible deformation. The shear stress required to initiate this mechanism is of the order of

$$\tau_Y = 2\mu(b/L) \quad (L \text{ is the length of the source})$$

a value much lower than the observed elastic limit;

in fact, due to the interatomic bonds broken at the core of dislocations, the so-called Peierls–Nabarro forces prevent the slip and give rise to a higher elastic limit;

the decomposition of dislocations leads to the creation of barriers which also restrict the slip;

the Frank networks offer a resistance to shear with an order of magnitude

$$\tau_Y = \frac{\mu b}{2\pi L} \quad (L \text{ is the length of the Frank cells});$$

in alloys, solid solutions or precipitates contribute to an increase in the resistance to dislocation movements.

Several of these mechanisms can occur simultaneously to give the values of elastic limit as measured macroscopically. In the case of polycrystals, the disorientation between the crystals and the grain boundaries, prevents the progress of irreversible deformation. Therefore, in this case we must add to the mechanisms described above a mechanism for crossing the grain boundary. By considering the equilibrium of forces due to the blocking of dislocations at the grain boundaries and those applied externally, and taking into account the fact that  $\tau_Y$ , the shear elastic limit, is the stacking stress in a crystal which can activate a dislocation source at a distance  $r$  in an adjacent crystal of mean length  $d$ , we obtain the following relation known as the Petch equation

$$\tau_y = \tau_0 + \tau^*(r/d)^{1/2}.$$

It is evident from this equation that the elastic limit varies in direct proportion to the square root of the distance  $r$ , and in inverse proportion to the square root of the average crystal length  $d$ ;  $\tau_0$  and  $\tau^*$  are coefficients which are characteristics of the metal or the alloy.

### *Deformation of polycrystals*

In order to define the basic assumptions of a model well, it is necessary to examine in a schematic way the sequence of mechanisms which occur in the deformation of a polycrystal during a uniaxial external loading, which first increases and then decreases (see Fig. 1.17).

*Elastic deformation (OY in Fig. 1.17)*

Elastic deformations result from reversible relative movements of atoms. They are almost independent of the permanent deformations except as regards the microscopic residual stresses which result from the irreversible crystalline slips causing the macroscopic elastic deformations to be slightly different from the sum of the microscopic elastic deformations.

*Elastic limit (Point Y in Fig. 1.17)*

The elastic limit is characterized by the state of stress or strain which causes the first irreversible movements of dislocations. As they are difficult to detect, we define the elastic limit or the yield stress,  $\sigma_Y$ , by convention to be the stress for a fixed amount of permanent strain;  $\epsilon^P = 0.02\%$  or  $0.05\%$  or  $0.2\%$  depending upon the precision required (see Chapter 5).

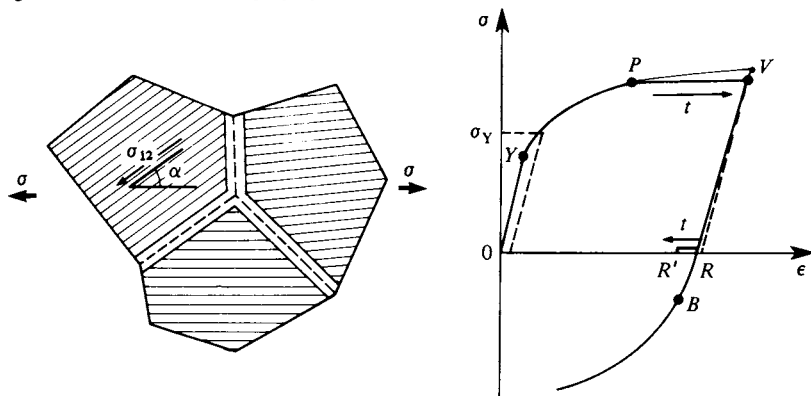
*Plastic deformation (YP in Fig. 1.17)*

The first slips occur in crystals with crystallographic slip planes oriented at  $\alpha = \pi/4$  to the direction of applied stress  $\sigma$ , where the shear stress  $\sigma_{12}$  is maximum. The reorientation of crystals, necessary to ensure compatibility of deformations, activates other slip systems and the deformation appears macroscopically homogeneous. It is a stable deformation and each state is that of an elastoplastic equilibrium.

*Hardening or consolidation (YP in Fig. 1.17)*

If the stress continues to rise, the dislocation density is increased but the number of barriers is increased even more, so that the deformation

Fig. 1.17. Deformation of a polycrystal.



cannot progress unless the load is increased. This increased resistance to slip deformation is the phenomenon of hardening which can also result from the presence of intercrystalline microstresses induced by the incompatibility of grain to grain deformations.

*Viscoplastic deformation (PV in Fig. 1.17)*

If the stress continues to rise, the slips can cross and follow the grain boundaries. This phenomenon of intergranular slip is favoured by thermal activation and is especially significant at temperatures higher than one third of the absolute melting temperature. A large part of the deformation, however, remains intragranular and is comprised of slip and climb of dislocations. When the deformation can progress under constant stress with no possibility of equilibrium, we have creep flow the rate of which depends on the applied stress; this is the domain of viscoplasticity.

*Restoration or recovery (RR' in Fig. 1.17)*

The modifications produced in an aggregate of polycrystals by deformation represent a deviation with regard to the thermodynamic equilibrium which tends to decrease under zero or reversed loading; the concentration of the vacancies or of the interstitial atoms decreases, dislocations of opposite signs neutralize each other, and recrystallization can occur. The recovery is a function of time and is favoured by thermal activation. On a macroscopic level, it manifests itself in a partial recovery of the deformation or in a decrease in the hardening. This description also applies to microstructurally stable materials. However, the phenomenon of ageing can occur which involves instabilities of structures or chemical compositions over a short or a very long time (e.g. ageing of some alloys after heat treatment).

*Plastic or viscoplastic incompressibility*

Since slip deformations do not alter the crystal structure, the total volume of an aggregate remains unchanged. Only elastic deformations produce a noticeable volume change; the change due to the increase of the density of dislocations, always remains very small. In the same way, a normal stress on the slip plane or a state of hydrostatic stress ( $\sigma_1 = \sigma_2 = \sigma_3$ ) has no effect on permanent deformations. This has been experimentally verified up to pressures of 30 000 atmos (3000 MPa).

*Anisotropy induced by permanent deformations*

As permanent deformations differ from one crystal to the next, the